The sum-over-histories formulation of quantum computing

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Abstract

Since Deutsch (1985), quantum computers have been modeled exclusively in the language of state vectors and the Schrödinger equation. We present a complementary view of quantum circuits inspired by the path integral formalism of quantum mechanics, and examine its application to some simple textbook problems.

1 Introduction

At the undergraduate level, quantum mechanics is usually taught in the so-called *canonical* or *Hamiltonian* formalism. In this formalism the state of a quantum system is given by a vector in a complex Hilbert space which evolves over time according to the Schrödinger equation, and measurable properties are modeled by Hermitian operators. The *path integral* or *Lagrangian* formalism is generally introduced at the graduate level in a first course in quantum field theory, though it is just as applicable to nonrelativistic quantum mechanics. In the path integral formalism there is no representation of the state of a quantum system between preparation and measurement. The probability of a transition between classical states is given by the integral, over every conceivable intermediate classical history of the system, of a complex-valued function of the history.

The canonical and path-integral approaches offer complementary views of the same quantum theory. Often problems which are very difficult to solve in one formalism are easy in the other: the path integral formalism is far better suited to calculating scattering amplitudes in high energy physics (with the help of Feynman diagrams), while the canonical formalism is far better for calculating energy levels of bound systems like the hydrogen atom.

Previous research in quantum computing seems to have used the canonical formalism exclusively. In this paper we attempt to remedy that oversight, by

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presenting a complementary view of quantum circuits inspired by the path integral formalism, and examining its application to some simple textbook problems.

2 From quantum mechanics to quantum circuits

2.1 Discretizing the canonical formalism

First we briefly review how the canonical formalism of continuum quantum mechanics is related to the discrete quantum circuit model. We write $|\psi\rangle$ for the state of a quantum system and say that it evolves in time according to the Schrödinger equation, $-i\hbar\frac{\partial}{\partial t}|\psi\rangle = H(t)|\psi\rangle$. Anticipating quantum circuits, we take the Hamiltonian H to be a function of time in order to model real-time classical control of the quantum system.

We first discretize the phase space by decreeing that our quantum system may only be in finitely many classical states. In the case of a quantum computer with n qubits there are 2^n states[1]; then $|\psi\rangle$ may be seen as a vector in a 2^n-dimensional space, or, with respect to the computational basis, as a $2^n \times 1$ column vector, each of whose components is a complex amplitude. The operator H becomes, with respect to the same basis, a $2^n \times 2^n$ matrix.

Next we discretize time, by supposing that the time between preparation and measurement is divided into finitely many intervals of length δt, and within each of these intervals H does not change. Then we can integrate the Schrödinger equation between t and $t+\delta t$, turning it into a difference equation,

$$|\psi_{t+\delta t}\rangle = e^{\frac{i}{\hbar}H(t)\delta t}\,|\psi_t\rangle\,.$$

It is easy to show that if H is Hermitian then e^{iH} is unitary; so $U = e^{-\frac{i}{\hbar}H(t)\delta t}$ is the unitary transition matrix that appears in the usual model of quantum circuits.

2.2 Discretizing the path-integral formalism

In the path-integral formalism, the quantum amplitude of a transition from a classical initial state at time t_i to a classical final state at time t_f is given by

$$A = \int \mathrm{D}\phi\; e^{\frac{i}{\hbar}S(\phi)}, \qquad \text{where} \qquad S(\phi) = \int_{t_i}^{t_f} \mathrm{d}t\; L(\phi(t), \dot{\phi}(t), t).$$

Here ϕ denotes a *history*, i.e. any conceivable sequence of classical states the system might occupy between t_i and t_f. The corresponding integral ranges over every possible history of the system, whether or not that history is permitted by classical laws of physics. The quantity $S(\phi)$ is the classical *action* associated with

[1]This is also true of classical computers, of course.

a particular history of the system, and L is the classical *Lagrangian*, which is a function of the state $\phi(t)$ and the rate of change of the state $\dot{\phi}(t)$ at a given time. Like the Hamiltonian, and for the same reason, we also give the Lagrangian an explicit time dependence. The relationship between the action and the Lagrangian survives unchanged from classical physics; the new physics is contained in the outer integral, which states that each history, even if classically absurd, contributes equally to the overall transition amplitude.

As before we discretize the path-integral formalism by limiting our system to 2^n classical states and dividing time into intervals of length δt. The histories ϕ become ordered tuples of states; each state requires n bits to describe, and each tuple contains $\Delta t/\delta t$ states (where $\Delta t = t_f - t_i$), so the outer integral becomes a sum over a discrete space of $2^{n(\Delta t/\delta t)}$ histories. The discretized Lagrangian depends on the current state and the difference between the current state and the next state, or equivalently on the current and next states directly. So we have (with suitable normalization) $A = \sum_\phi \exp\left(\frac{i}{\hbar}\sum_{t=t_i}^{t_f} L(\phi_t, \phi_{t+\delta t}, t)\right)$. Finally we move the exponential inside the sum, obtaining

$$A = \sum_\phi \prod_{t=t_i}^{t_f} B(\phi_t, \phi_{t+\delta t}, t)$$

where $B(\cdots) = e^{\frac{i}{\hbar}L(\cdots)}$.

We will refer to the discretized path-integral formalism as the *sum-over-histories* formalism.

2.3 Equivalence of the canonical and sum-over-histories formalisms

There is a delightfully simple way to see that the discrete canonical and sum-over-histories formalisms are mathematically equivalent. In the canonical formalism we start with a system prepared in the state $|\psi_0\rangle$, which we may assume to be an eigenstate of the computational basis. To this we apply a sequence of unitary transformations, obtaining $|\psi_1\rangle = U^{(1)}|\psi_0\rangle, \ldots, |\psi_m\rangle = U^{(m)}|\psi_{m-1}\rangle$. Finally we measure all of the qubits, obtaining the computational eigenstate $|\psi_f\rangle$ with probability $|\langle\psi_f|\psi_m\rangle|^2$. Combining these steps into one, we have that the probability is the squared modulus of $A = \langle\psi_f|U^{(m)}\cdots U^{(1)}|\psi_0\rangle$. Writing out the matrix product explicitly,

$$A \quad = \quad \sum_{i_1}\cdots\sum_{i_{m-1}} U^{(m)}_{i_m i_{m-1}}\cdots U^{(2)}_{i_2 i_1} U^{(1)}_{i_1 i_0} \quad = \quad \sum_{i_1}\cdots\sum_{i_{m-1}}\prod_{j=1}^{m} U^{(j)}_{i_j i_{j-1}}$$

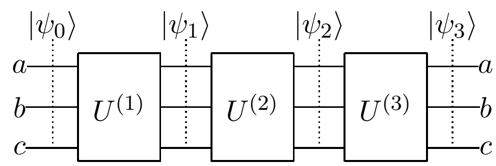
where each sum is taken over the 2^n states of the computational basis, and i_0 and i_m are the initial and final basis states $|\psi_0\rangle$ and $|\psi_f\rangle$. But this is exactly the sum

over histories, with $\phi = (i_1, \ldots, i_{m-1}) \in (2^n)^{m-1}$ and $B(\phi_{j-1}, \phi_j, t) = U^{(j)}_{i_j i_{j-1}}$.[2]

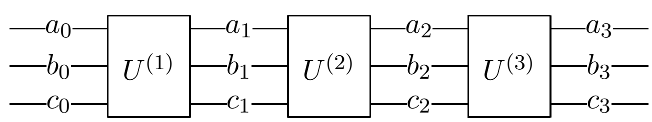
3 Quantum circuits in the sum-over-histories picture

The reader may be wondering at this point why we bothered to introduce the sum-over-histories formalism, if its difference from the canonical formalism amounts to mere algebra. In this section we justify its existence by showing that it leads to an interesting new view of quantum circuits.

Returning to the canonical formalism for the moment, consider a small quantum system of three qubits (call them a, b and c) to which we successively apply three unitary transformations, transforming the system through two intermediate states to a final state. We might illustrate this as follows:



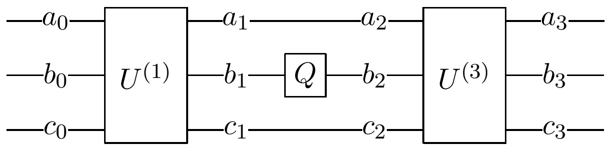
In the sum-over-histories formalism we never deal with general state vectors, only with classical states—i.e. computational basis vectors—so instead of $|\psi_0\rangle, \ldots, |\psi_3\rangle$ we may as well write $|a_0 b_0 c_0\rangle$, ..., $|a_3 b_3 c_3\rangle$, with each a_k, b_k, c_k taking on a value from $\{0, 1\}$ in a particular history. In fact, there is no need to write these variables in a ket above the circuit: it is clearer to place them on the wires themselves.



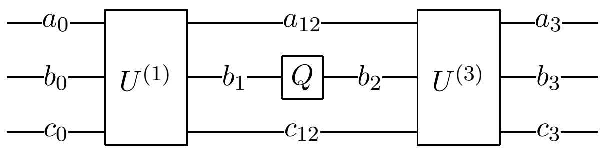
So if the system is prepared in the state $i_0 = |a_0 b_0 c_0\rangle$, the amplitude that it will be found in the state $i_3 = |a_3 b_3 c_3\rangle$ after application of these three unitary gates can be found by summing the contribution of the $2^6 = 64$ histories arising from all possible choices of $a_1, b_1, c_1, a_2, b_2, c_2 \in \{0, 1\}$. The contribution of each history is the product $U^{(1)}_{|a_1 b_1 c_1\rangle |a_0 b_0 c_0\rangle} U^{(2)}_{|a_2 b_2 c_2\rangle |a_1 b_1 c_1\rangle} U^{(3)}_{|a_3 b_3 c_3\rangle |a_2 b_2 c_2\rangle}$. Clearly this extends to any number of gates; it merely paraphrases the explicit formula of Section 2.2.

[2]In fact we have glossed over a serious problem here: the derivation of section 2.2 implies that the modulus of B is independent of its arguments, and this certainly is not true of the components of the matrices U. To actually obtain arbitrary unitary matrices from the path-integral formalism we must further subdivide δt. But for the purposes of this section it is enough to simply generalize B.

Suppose now that $U^{(2)}$ acts only on qubit b—i.e. that $U^{(2)} = I \otimes Q \otimes I$, where $I = \left(\begin{smallmatrix}1&0\\0&1\end{smallmatrix}\right)$ and Q is some 2×2 unitary matrix.

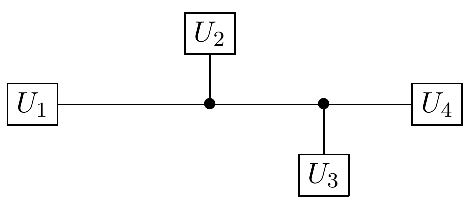


Most of the entries of $U^{(2)}$ are now zero; specifically, $U^{(2)}_{|a_2b_2c_2\rangle|a_1b_1c_1\rangle} = I_{a_2a_1}Q_{b_2b_1}I_{c_2c_1}$, which is zero at least when $a_1 \neq a_2$ or $c_1 \neq c_2$. Therefore, the total contribution of any history with $a_1 \neq a_2$ or $c_1 \neq c_2$ will be zero. Therefore, we need not consider those histories at all! We can easily exclude them by taking $a_1 = a_2 = a_{12}$ and $c_1 = c_2 = c_{12}$.

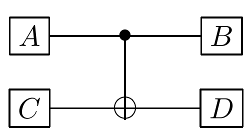


Now we may compute the same transition amplitude as before by summing the contribution of just 16 histories arising from all possible choices of $a_{12}, b_1, b_2, c_{12} \in \{0, 1\}$.

Generalizing this idea, we arrive at the following formulation of sum-over-histories for quantum circuits. We say that an *internal wire* begins as the output of a gate and ends as the input to another gate, possibly controlling other gates along the way. For example, this is an internal wire:



This is three internal wires (one above, two below):



An *external wire* begins as an input to the circuit and ends at a gate, or begins at a gate and ends as an output from the circuit, or begins as an input and ends as an output. Like an internal wire, it may control other gates along the way.

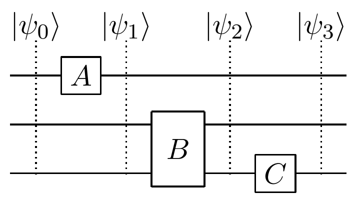
We assign a value of either 0 or 1 to each internal and external wire in every possible way. The values of the external wires are fixed by the specification of

the inputs and outputs of the circuit, while the values of the internal wires are not; thus there are 2^w possible assignments (histories), where w is the number of internal wires. For each of these histories, for each gate in the circuit, we find the element of the unitary matrix indexed by the inputs and outputs of the gate. We multiply these to find the contribution of the history, and add the contributions of every history to find the transition amplitude, whose squared modulus is the transition probability.

Note that even though our new history-enumeration rule eliminates all zeroes that arise from tensor products with the identity, there may still be zeroes lurking within our gates. We will say that a gate *rejects* a history if it causes that history's contribution to go to zero. A gate defined by a matrix containing only ones and zeroes will either reject a particular history or contribute a factor of one, effectively doing nothing (which we will call *accepting* the history). A gate which either accepts or rejects every history is *classical*.

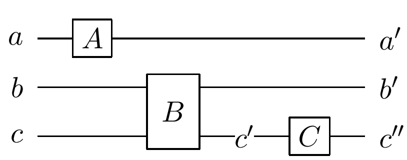
3.1 Topological quantum computing

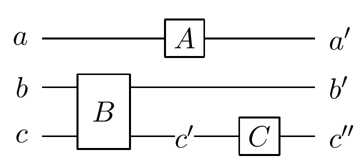
Returning to the canonical formalism, consider the circuit



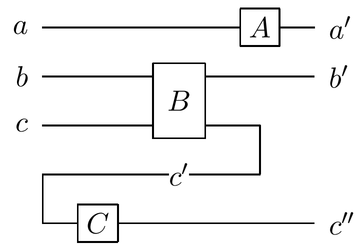
It is of course true (though not immediately obvious in this formalism) that we may switch the order of gates A and B in this circuit without affecting the subsequent states ($|\psi_2\rangle$ and $|\psi_3\rangle$). But state $|\psi_1\rangle$ does change: in the revised circuit it is replaced by an entirely different state (call it $|\psi_1'\rangle$). There is no straightforward relationship between $|\psi_1\rangle$ and $|\psi_1'\rangle$.

If we apply sum-over-histories to this circuit, it is immediately clear that A and B may be switched without affecting the result; it is equally clear that *nothing changes* when we switch them, not even unobservable bookkeeping state.





Circuits are in some sense topological in the sum-over-histories picture. We do not have any state which cuts across all wires, imposing a linear order on our gates. Indeed, it is not clear that we cannot use sum-over-histories to find a transition amplitude for a circuit like



which has no obvious interpretation at all in the canonical formalism.

Some care is necessary here because many gates are not symmetric with respect to rearrangement of their parameters. If we were to move the C gate to the location of the c' wire label, we would have to indicate somehow that its left and right parameters had switched places. An obvious solution is to write C^t instead of C in this situation (note that this is the transpose, not the adjoint). Fortunately, many common gates turn out to be perfectly symmetric, and here we will look at three interesting examples.

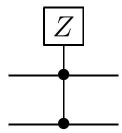
First, the CNOT gate, which we now view as a three-parameter gate, accepts every history where the sum of its parameters is even, and rejects all other histories. So it is in fact perfectly symmetric between "input," "output," and "control," and we need not distinguish them at all. We will call the symmetric version of CNOT the *xor gate*.

Second, diagonal gates like Z and $\pi/8$, which we will here call *phase gates*, are perfectly symmetric between input and output. In fact, the input and output are actually the same wire: the off-diagonal zeroes cause rejection of any history in which they carry different values. Another way to see this is to look at the sequence controlled-controlled-Z, controlled-Z, Z:

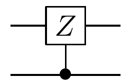
$$\begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & -1 \end{pmatrix}, \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix}, \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

It is clear that this sequence has been cut off one term short of its natural end. The next term ought to be (-1), a unitary 1×1 *zero*-qubit gate which we will call the *–1 gate*. The same applies to any single-qubit gate described by a diagonal matrix. These gates actually operate on no qubits at all; for consistency we should

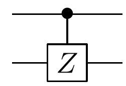
write



instead of



or



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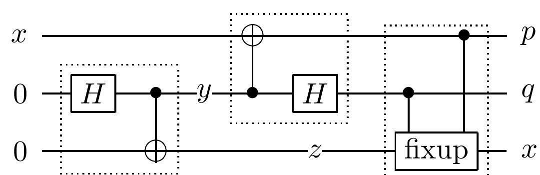
A free-floating (uncontrolled) phase gate contributes the same phase to every history, which has no observable effect.

Third, the uncontrolled Hadamard gate does not reject any combination of input and output; if both of its parameters are 1 it contributes a factor of -1 to the history; and regardless of its parameters it contributes an additional factor of $\frac{1}{\sqrt{2}}$. We can absorb the factor of $\frac{1}{\sqrt{2}}$ into a post-normalization step, since it is the same for every history. Without this factor, the effect of the Hadamard gate is exactly that of the controlled-Z gate. So the Hadamard gate is nothing but a doubly-controlled -1 gate which just happens to be written with its control wires on the left and right instead of the top and bottom.

It is well known that classical gates plus H, Z and $\pi/8$ constitute a universal quantum gate set. We have just shown that in the sum-over-histories formalism H, Z and $\pi/8$ are all special cases of the controlled zero-qubit phase gate. The extra power of quantum computers seems to be vested entirely in gates that do not affect any qubits!

4 Case study: quantum teleportation

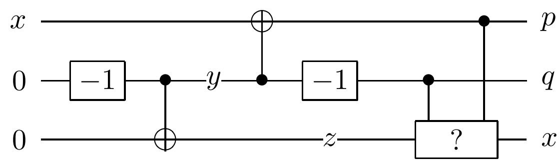
Here is a typical quantum teleportation circuit.



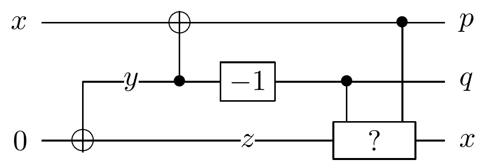
The boxes mark the three conceptually separate parts of this circuit; left to right, they are the Bell state creation (performed jointly by Alice and Bob), the Bell state uncreation (performed by Alice), and the "fixup" step (performed by Bob with two bits of classical information from Alice).

The question that interests us here is, what is the $\boxed{\text{fixup}}$? Working this out from the state vector is tedious. In this section we will see how to find the answer from the sum over histories without any calculation at all.

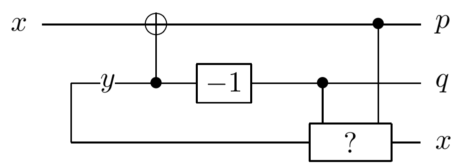
We begin by replacing Hadamard gates with doubly-controlled -1 gates.



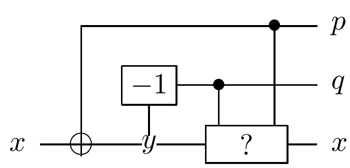
One of the controls for the first -1 gate is always 0, so the gate will never be active. We can simply drop it:



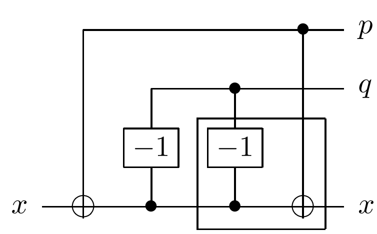
At the lower left we have an xor gate one of whose parameters is always zero. Under these circumstances, the gate will accept a circuit iff its other two parameters are equal. So we may as well short those parameters together: y and z are the same wire.



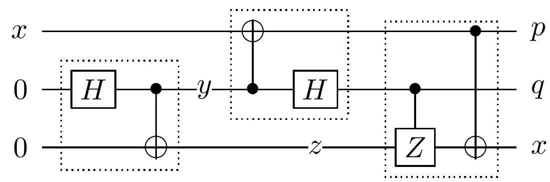
A bit of rearrangement gives



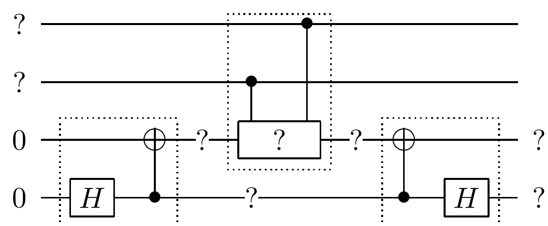
The situation, then, is as follows: if p, then $y = \neg x$, otherwise $y = x$; and if $q \,\&\, y$, then the whole world has been rotated by $180°$ in the complex plane. The job of the ? is to undo the rotation and recover x, and it is now easy to see how to do this.



Backporting this result to the conventional notation gives us the solution to the original problem.



With a bit of practice it is possible to perform all of these steps mentally, reading the answer directly off of the original circuit. As an exercise, the reader might try to find the correct fixup step for this closely related superdense coding circuit, and also label the marked wires with p, q, x, y, and z according to their correspondence to the wires in the diagram above.



5 Conclusions

Is the sum-over-histories formalism useful? Path-integral techniques in physics have been fantastically successful, but it is not clear that this is relevant to quantum computing. In physics one is often interested in calculating quantum corrections to a roughly classical quantity, while in quantum computing one generally wants to be as far from classical behavior as possible. The QFT, the key to so many quantum algorithms, is in a certain sense maximally nonclassical. Probably there will be no polynomial-time circuit simulation algorithms forthcoming from the sum-over-histories formalism.

Sum-over-histories certainly gives a useful perspective on some results in complexity theory. The fact that **BQP** $\subseteq$ **PSPACE**, surprising in the canonical formalism, is almost self-evident in sum-over-histories. A naïve circuit simulator based on sum-over-histories requires very little space, especially compared to the exorbitant requirements of a state-vector simulator. Of course, all of this is well known already.

This author's particular interest is language design, and he has some hope that sum-over-histories might be useful here. What properties would we expect of a language which compiles to a "topological" quantum circuit, in the sense of Section 3.1, instead of a sequential circuit? A serious complication is that it is not clear how to go backwards from a topological circuit to something actually

realizable on quantum hardware. It would be necessary to find an algorithm which not only recovers a circuit, but recovers it quickly enough that it is not faster to simply simulate the topological circuit classically. Worse, only some topological circuits correspond to any realizable circuit, and it is not clear how to characterize these.

The author is particularly hopeful that sum-over-histories could be useful in education. It is a truism that one has not understood something until one has understood it in two different ways. Many textbooks, as well as popular introductions to quantum mechanics, foster the impression that the state vector is *really* the state of a quantum system, and the universe really is keeping track of 2^n complex amplitudes. In fact there are good theoretical reasons not to take state vectors too seriously as a model of physical reality. It might also be easier in the sum-over-histories picture to motivate the connection between classical and quantum computing, and the embedding of the former in the latter. The notion of classical gates "accepting" and "rejecting" histories is reasonably intuitive, and a circuit containing only classical gates rejects all histories but one.